UCRL-JC-121531 Abs

Submitted to Symposium : V
Symposium Title : Scientific basis for nuclear waste management

ASSESSMENT OF DATABASES USED TO CALCULATE WATER-CEMENT-CO_2 INTERACTIONS AT ELEVATED TEMPERATURES USING EQ3/6 GEOCHEMICAL MODELING CODE

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Cementitious materials may play an important role in the disposal of radioactive waste. Low-level wastes can be encapsulated directly in cement. In this case, the cementitious material is not expected to experience elevated temperatures. High level radioactive waste (HLRW) is not intended for storage in cement, but rather in more robust metal or ceramic packaging. However, significant quantities of cement may be used (e.g. rock consolidation and invert emplacement) as part of HLRW repository construction. These materials may experience elevated temperatures for extended periods of time, due primarily to radioactive decay heat. Our study particularly concerns the ability to simulate chemical interactions between groundwater and cementitious construction materials in a HLRW repository environment. Specifically, our study is used to determine whether the available thermodynamic databases are adequate and internally consistent for simulations of chemical reactions that include crystalline calcium silicate hydrate phases at elevated temperatures. To that end, a series of modeling exercises was designed to simulate the dissolution of selected cement phases for temperature conditions ranging from 25°C to roughly 90°C. Two extreme scenarios were investigated: a) open system - fixed pCO_2 at approximately atmospheric values, (representing the free flow of atmospheric air through both the ventilation system and the rock fracture network of the repository; and b) closed system - evolving pCO_2 with reaction progress (representing the absence of ventilation as might be the case in a non-ventilated waste emplacement drift). For each of these scenarios, the evolution of J-13 well water and other water compositions that represent a range of pH and salinity conditions, have been simulated.

Work performed under the auspices of the Yucca Mountain Site Characterization Project (YMP) and a USDOE/AECL (Canada) International Agreement as part of the Civilian Radioactive Waste Management Program by Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.